The development of novel optical screening tests for the presumptive identification of New Psychoactive Substances (NPS) in seized illicit materials

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University of Technology Sydney

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Certificate of original authorship

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- Charles Dickens, Tale of Two Cities, 1859

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Abbreviations

^{13}C-NMR	carbon nuclear magnetic resonance
^{1}H-NMR	proton nuclear magnetic resonance
4-EMC	4-ethylmethcathinone
4-FMC	4-fluoromethcathinone
4-HMC	1-(4-hydroxyphenyl)-2-(methylamino)propan-1-one
4-MEC	4-methylethcathinone
4-MMC	4-methylmethcathinone
4-MPBP	1-(4-methylphenyl)-2-(pyrrolidin-1-yl)butan-1-one
4-MPPP	4-methylpyrrolidinopropiophenone
AC	alternating current
ACN	acetonitrile
amu	atomic mass unit
approx.	approximately
aq.	aqueous
atm	atmosphere
ATR	attenuated total reflectance
br.	broad
BuMgCl	butylmagnesium chloride
CAT	2-amino-1-phenylpropan-1-one
conc.	concentrated
d	doublet
DCM	dichloromethane
dd	doublet of doublet
dec.	decomposed
deform.	deformation
EI	electron ionisation
Et2O	diethyl ether
EthMgCl	ethylmagnesium chloride
FTIR	Fourier transform infrared
GC-MS	gas chromatography-mass spectrometry
h	hours
J	coupling constant

lit.	literature value
M	moles per litre
m	multiplet
m/z	mass to charge ratio
M+	molecular ion
MCAT	methcathinone
MDPBP	1-(2H-1,3-benzodioxol-5-yl)-2-(pyrrolidin-1-yl)butan-1-one
MDPBP	1-(2H-1,3-benzodioxol-5-yl)-2-(pyrrolidin-1-yl)butan-1-one
MDPV	3,4-methylenedioxypyrovalerone
MDPV	3,4-methylenedioxypyrovalerone
MeOH	methanol
min	minutes
MIP	molecularly imprinted polymer
MIPH	molecularly imprinted photonic hydrogels
MOMV	1-(4-methoxyphenyl)-2-(methylamino)pentan-1-one
mp	melting point
MW	molecular weight
NPS	new psychoactive substance
ø	diameter
oop	out of plane
PCC	pyridinium chlorochromate
PE	polyethylene
ppm	parts per million
ppt.	precipitate
PropMgCl	propylmagnesium chloride
PVAc	polyvinyl acetate
q	quartet
RBF	round bottom flask
Ref.	references
R_f	retardation factor
RT	room temperature
s	singlet
SN_2	one step nucleophilic substitution reaction
t	triplet
THF	tetrahydrofuran

TIC	total ion chromatogram
TLC	thin layer chromatography
TMS	tetramethylsilane
UCNP	upconversion nanoparticles
unk.	unknown
unsym.	unsymmetrical
UV-Vis	ultraviolet-visible
α-PVP	α-pyrrolidinopentiophenone
δ	chemical shift
λ	wavelength
$\bar{\nu}$	wavenumber

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Abstract

The large and increasing number of illicit materials seized each year combined with the introduction of many new psychoactive substances (NPS) to the traditional drug market are concerning realities. The need for simple presumptive field tests able to accurately detect compounds such as synthetic cathinones with good sensitivity is apparent. Field testing is an important tool for law enforcement officers to obtain rapid feedback regarding an unknown substance while awaiting confirmatory analysis results often in a backlog.

Chemical reactions selective toward the synthetic cathinone molecular structure were investigated for their application as a receptor element in an optical screening test. Oximations, hydrazone formations, semicarbazide formations and metal complexation were examined with a number of cathinone analogues. As an alternative to chemical reactions, molecularly imprinted polymers (MIPs) selective toward synthetic cathinone compounds were prepared, optimised and tested for their selective binding ability.

The synthetic cathinone class of compounds failed to show significant reactivity with the reagents selected under a range of experimental conditions. However, their ability to actively reduce the cupric ion of a copper-neocuproine complex to afford a yellow-orange coloured product was observed. This colour test was optimised, validated and later improved upon to increase useability in the field as an optical screening test. The MIPs showed potential in selectively recognising the presence of the target cathinone molecule through binding studies performed, however, before the polymer can be used as a receptor, further optimisation is required.

The three receptors investigated provided different degrees of success. The chemical colour test was successfully developed into a protocol for application in field testing of cathinones; the MIPs showed some potential for further investigation and application in a different protocol for cathinone detection; and the use of chemical reactions for tagging purposes was not achieved due to the inherently unreactive carbonyl group of the cathinone molecular structure. Nonetheless, this research provided significant and useful chemical analysis of the synthetic cathinone class of NPS, while raising awareness of current deficiencies in the presumptive identification of NPS.

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Chapter 1: Introduction

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